

Statistical properties of 1D spin glasses from first principles of classical mechanics

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Abstract

We study the classical 1D Heisenberg spin glasses, assuming that the orientation of spins are a spatial. The system of *recurrence equations* (RE) is obtained, by minimization of the nearest-neighbor Hamiltonian in nodes of 1D lattice. It is shown that in each node of the lattice there is a probability of bifurcation of the solution of REs. This leads to the fact that, performing a consecutive node-by-node calculations on the n -th step instead of a single stable spin-chain we get a set of spin-chains (strings) which form Fibonacci subtree (graph). Assessing the computational complexity of one graph shows that it is $\propto 2^n K_s$, where n and K_s denote the subtree height and Kolmogorov's complexity of a string respectively. It is shown that the statistical ensemble may be represented as a set of random graphs, where the computational complexity of each graph is \mathbb{NP} hard. It is proved, that all strings of the ensemble have the same weights. This allows in the limit of statistical equilibrium, with a predetermined accuracy to reduce the initial \mathbb{NP} hard problem to the \mathbb{P} problem. As shown, the statistical distributions of different parameters, which are performed by using \mathbb{NP} and \mathbb{P} algorithms for the respective curves provide a perfect coincidence. Lastly using the formal similarity between the ergodic dynamical system and ensemble of spin-chains, a new representation for the partition function in the form of one dimensional integral from the spin-chains energy distribution is proposed.

I. INTRODUCTION

A wide class of phenomena in physics, chemistry, material science, biology, nanoscience, neural network, evolution, organization dynamics, hard-optimization, environmental and social structures, human logic systems, financial mathematics etc, mathematically are well described by models of spin glasses¹⁻¹⁰. Despite numerous studies nonetheless there are still a number of topical issues in the field of spin glasses and disordered systems as a whole, the solution of which is extremely important from the point of view of the development of modern technologies. We can mention important ones of them;

a) The simulation of spin glasses far from thermodynamic equilibrium. It is obvious, in such cases, we can not enter the ambient temperature and, respectively, write and use a standard representation for partition function.

b) Even if it is assumed that spin glass is in the state of the thermodynamic equilibrium, and for it may be written in the standard form the partition function, in the frameworks of standard theoretical and numerical methods, it remains an open research question of metastable states. Recall that the Monte Carlo simulation methods allow us to study the spin systems only in the *ground state*, at the time when the real statistical system, all the more spin glasses, always are in the metastable states, i.e in the state where characterizing the spin glass parameters have some distributions.

c) At definition of the partition function, a priori is assumed that the total weight of nonphysical spin configurations in the configuration space is a zero that in a number of cases may be an incorrect assumption. Recall that under the nonphysical spin configurations, we mean such spin-chains, which are unstable based on the basic principles of classical mechanics.

d) The computational complexity of spin glasses often applies to the class of the \mathbb{NP} hard problems. This circumstance to require the development of new efficient algorithms for a numerical simulation of spin glasses that one way or another leads to the problem of reduction of the \mathbb{NP} hard to the \mathbb{P} problem.

As it was shown in works¹¹⁻¹⁴, the problem of spin glasses even in the state of the thermodynamic equilibrium often are \mathbb{NP} hard problems, whose source of which is in the diverging equilibration at simulations by the Monte Carlo methods¹⁵. In the last time in the statistical physics occurs a rapid growth the number of works on methods of the com-

binatorial optimization^{16–18}. In particular a number of disordered statistical systems have been mapped onto combinatorial problems, for which a fast combinatorial optimization algorithms are available^{19,20}. So, combinatorial methods and corresponding algorithms are often used for a simulation of spin glasses especially when studying the phenomena such as phase transitions where they have given valuable insights about questions that are hard to investigate by traditional techniques, for example by Monte Carlo simulations¹¹. However, the above-mentioned questions, on which we want to obtain clear answers, obviously, require to development of principally new approaches.

In this paper we will study the classical 1D spin glass problem suggesting that only the nearest neighboring spins interact. Recall despite the simplicity of the model, since in a known sense it's an exactly solvable model²¹, as it will shown below, all the aforementioned problems in this model are present, if we try to solve the task from first principles of classical mechanics.

One of the important goals of this work is to prove, that in the limit of statistical equilibrium the initial NP-hard problem with the prescribed accuracy can be reduced to the \mathbb{P} problem, that in turn implies the creation of high-performance algorithm for simulation of the Heisenberg type spin glasses. In the work possibilities of generalization of the model for descriptions of more complex and realistic disordered systems of nature are also discussed.

II. DEFINITION OF MODEL

The disordered 1D spin-chain in the framework of the nearest-neighboring Heisenberg model may be written as:

$$H = - \sum_{i \in \mathcal{N}} J_{i,i+1} \mathbf{s}_i \mathbf{s}_{i+1}, \quad \mathbf{s}_i \in \mathbb{R}^3, \quad \|\mathbf{s}_i\| = \|\mathbf{s}_{i+1}\| = 1, \quad (1)$$

where $\mathcal{N} = \{1, \dots, n\}$ is the set of nodes on 1D lattice, the couplings $J_{i,i+1}$ are independent random variables characterizing the power of interactions between spins. The distribution of the coupling constants will be found below as a result of the numerical simulation.

Since the norm of vector $\mathbf{s}_i = (x_i, y_i, z_i)$ is equal to the unit, then the projection, z_i can be represented in the following form:

$$z_i = q_i |z_i|, \quad z_i = (1 - x_i^2 - y_i^2)^{1/2} > 0, \quad q_i = \text{sign}(z_i), \quad (2)$$

where q_i is a discrete variable which can take two possible values +1 and -1.

Substituting the Hamiltonian (1) into Hamilton equations (see for example²²) can be found:

$$\begin{aligned} -\ddot{x}_i &= J_{i-1,i}(x_{i-1} - x_i z_i^{-1} z_{i-1}) + J_{i,i+1}(x_{i+1} - x_i z_i^{-1} z_{i+1}), \\ -\ddot{y}_i &= J_{i-1,i}(y_{i-1} - y_i z_i^{-1} z_{i-1}) + J_{i,i+1}(y_{i+1} - y_i z_i^{-1} z_{i+1}), \end{aligned} \quad (3)$$

where the following notations are made, $\ddot{\xi}_i = \partial^2 \xi_i / \partial t^2$ and $\xi = (x, y)$, in addition "t" denotes the usual time. We will assume that near the nodes spins are localized and quasi-periodic movements commit, $\xi_i(t) = \xi_i^0 + \delta_i^\xi(t)$, where ξ_i^0 and $\delta_i(t)$ denote the position of the equilibrium and quasi-periodic function of the time respectively. Below we will study the statistical properties of the system, which are formed on time scales $\tau \gg \tau_0$, where τ_0 is a characteristic time of spins oscillation and obviously, in this case; $\langle \ddot{x} \rangle_{\tau_0} = \langle \ddot{y} \rangle_{\tau_0} \approx 0$. Averaging equations (3) on the period τ_0 can be found:

$$\begin{aligned} J_{i-1,i}(x_{i-1} - x_i z_i^{-1} z_{i-1}) + J_{i,i+1}(x_{i+1} - x_i z_i^{-1} z_{i+1}) &= 0, \\ J_{i-1,i}(y_{i-1} - y_i z_i^{-1} z_{i-1}) + J_{i,i+1}(y_{i+1} - y_i z_i^{-1} z_{i+1}) &= 0, \end{aligned} \quad (4)$$

where for simplicity in equations the index "0" over of variables are omitted, i.e $x_i^0 \rightarrow x_i$, $y_i^0 \rightarrow y_i$ and $z_i^0 \rightarrow z_i$. As it is easy to verify these equations define the condition at which the Hamiltonian (1) in the i -th node takes extremal value.

Solving the system of equations (4), with respect to the variables x_{i+1} and y_{i+1} , it can be found:

$$x_{i+1} = C_x / J_{i,i+1}, \quad y_{i+1} = C_y / J_{i,i+1}, \quad (5)$$

where the following notations are made:

$$C_{x(y)} = \frac{A_{x(y)} - B_{y(x)}(C \pm \sqrt{D})}{1 + B_x^2 + B_y^2}, \quad A_\eta = \eta_i z_i^{-1} z_{i-1} - \eta_{i-1}, \quad B_\eta = \eta_i z_i^{-1} z_{i+1},$$

$$D = (1 + B_x^2 + B_y^2 - A_x^2 - A_y^2 - C^2) > 0, \quad C = A_x B_y - A_y B_x, \quad \eta = (x, y).$$

Now, for the Hamiltonian (1) we can formulate conditions of the local minimum. It is obvious that i -th spin is in the stable equilibrium, if in the stationary point the following inequalities are satisfied:

$$A_{x_i x_i}(\mathbf{s}_i^0) > 0, \quad A_{x_i x_i}(\mathbf{s}_i^0) A_{y_i y_i}(\mathbf{s}_i^0) - A_{x_i y_i}^2(\mathbf{s}_i^0) > 0, \quad (6)$$

where $A_{\eta_i \eta_i} = \partial^2 H / \partial \eta_i^2$ and $A_{x_i y_i} = \partial^2 H / \partial x_i \partial y_i$; in addition \mathbf{s}_i^0 denotes i -th spin which is in a stable equilibrium.

Using (2), (4) and (6), we can calculate the explicit forms of the second order derivatives:

$$A_{\eta_i \eta_i} = (\eta_i^2 + z_i^2) z_i^{-3} \Delta_i, \quad A_{x_i y_i} = x_i y_i z_i^{-3} \Delta_i, \quad \Delta_i = (J_{i-1, i} z_{i-1} + J_{i+1, i} z_{i+1}), \quad (7)$$

and taking into account (6) and (7), it is easy to find the conditions for a local minimum of energy:

$$A_{x_i x_i} = (1 - y_i^2) z_i^{-3} \Delta_i > 0, \quad A_{x_i x_i} A_{y_i y_i} - A_{x_i y_i}^2 = z_i^{-4} \Delta_i^2 > 0. \quad (8)$$

Since by definition (2) $z_i > 0$, then both of the conditions in (8) are satisfied:

$$\Delta_i = (J_{i-1, i} z_{i-1} + J_{i+1, i} z_{i+1}) > 0. \quad (9)$$

Thus, in each node the solutions defining the orientation of the spin in the state of the local equilibrium can be found, if we find such coupling constants $J_{i, i+1}$, for which not only conditions (8) or (9) are satisfied, but also holds the inequality:

$$J_{i, i+1}^2 \geq C_x^2 + C_y^2 > 0. \quad (10)$$

As will be shown below, the additional condition (10) will play an important role at simulation.

III. GEOMETRIC PROPERTIES OF DISORDERED 1D SPIN-CHAIN

Theorem. *If the set of spatial spins; $\{\mathbf{s}\} = (\mathbf{s}_1, \dots, \mathbf{s}_n)$ forms the stable 1D spin-chain (see conditions (8)) then they necessarily are coplanar in the sense, that at parallel moving to the origin all spins lie in the same plane.*

Proof. Let us consider the three consecutive spatial spins \mathbf{s}_{i-1} , \mathbf{s}_i and \mathbf{s}_{i+1} on the 1D lattice. If we join the origins of two consecutive spins \mathbf{s}_{i-1} and \mathbf{s}_i , they will form a plane Λ_0 . In this connection arises the question namely as subsequent spins are oriented relative to the plane Λ_0 ? Since these spins are in the positions of local minima, we can use the system of equations (4) for defining bonds between projections of three nearest-neighboring spins. In particular, from the first equation in (4) for the solution z_{i+1} , we can find the following expression:

$$z_{i+1} = \frac{J_{i-1, i} (x_{i-1} z_i - x_i z_{i-1}) + J_{i, i+1} x_{i+1} z_i}{J_{i, i+1} x_i}. \quad (11)$$

Substituting z_{i+1} into the second equation in (4), the expression of bond between projections of two spins \mathbf{s}_{i-1} and \mathbf{s}_i can be found:

$$x_{i-1}y_i - x_iy_{i-1} = \frac{J_{i,i+1}}{J_{i-1,i}}(x_{i+1}y_i - x_iy_{i+1}). \quad (12)$$

The spin \mathbf{s}_{i+1} is a parallel to the plane Λ_0 , if the following equation is satisfied:

$$\begin{vmatrix} x_{i-1} & y_{i-1} & z_{i-1} \\ x_i & y_i & z_i \\ x_{i+1} & y_{i+1} & z_{i+1} \end{vmatrix} = 0. \quad (13)$$

We can write the equation (13) in the explicit form:

$$\det |\cdot| = x_{i-1}y_i z_{i+1} + x_{i+1}y_{i-1} z_{i+1} + x_i y_{i+1} z_{i-1} - x_{i+1}y_i z_{i-1} - x_i y_{i-1} z_{i+1} - x_{i-1}y_{i+1} z_i =$$

$$x_{i+1} \left[-\frac{J_{i,i+1}}{J_{i-1,i}}(y_{i+1} z_i - y_i z_{i+1}) \right] + y_{i+1} \left[\frac{J_{i,i+1}}{J_{i-1,i}}(x_{i+1} z_i - x_i z_{i+1}) \right] + z_{i+1} \left[-\frac{J_{i,i+1}}{J_{i-1,i}}(x_{i+1} y_i - x_i y_{i+1}) \right],$$

Finally, using the expression (12) it is easy to show that:

$$\det |\cdot| = \frac{J_{i,i+1}}{J_{i-1,i}} \left\{ x_{i+1}(y_i z_{i+1} - z_i y_{i+1} - y_i z_{i+1} + z_i y_{i+1}) + x_i(y_{i+1} z_{i+1} - y_{i+1} z_{i+1}) \right\} = 0.$$

Thus the theorem is proved.

Note that, the specified geometric property allows simplifying the Hamiltonian (1).

Let us consider the set of spins in the spherical coordinate system $(\alpha_i, \theta_i, \vartheta_i)$. In the new coordinates for two consecutive spins, we can write the following relationship:

$$\mathbf{s}_i \mathbf{s}_{i+1} = \|\mathbf{s}_i\| \cdot \|\mathbf{s}_{i+1}\| = \cos(\alpha_i - \alpha_{i+1}), \quad (14)$$

where $(\alpha_i, \alpha_{i+1}) \in [-\pi, +\pi]$ are angles of the respective spins in planes parallel to plane Λ_0 .

Using (14) Hamiltonian (1) can be written as:

$$H = -P(\theta, \vartheta) \sum_{i=1}^n J_{i,i+1} \cos(\alpha_i - \alpha_{i+1}), \quad (15)$$

where, as it follows from the proof of the proposition, $\theta = \theta_1 = \dots = \theta_n \in (-\pi, +\pi]$ and $\vartheta = \vartheta_1 = \dots = \vartheta_n \in [0, \pi]$. In addition, the pair of angles (Θ, ϑ) determines the orientation of the plane Λ_0 in 3D space. It is natural to propose that $P(\theta, \vartheta)$ is a homogeneous distribution function from angles, which is normalized on unit $\int \int P(\theta, \vartheta) d\theta d\vartheta = 1$.

For finding the extreme value of the Hamiltonian (15) in nodes, let us consider the first derivative by the angle α_i :

$$\frac{dH}{d\alpha_i} = P(\theta, \vartheta) [J_{i-1,i} \sin(\alpha_{i-1} - \alpha_i) - J_{i,i+1} \sin(\alpha_i - \alpha_{i+1})]. \quad (16)$$

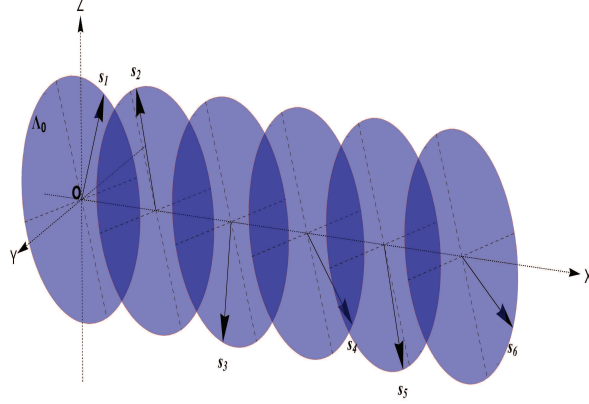


FIG. 1. *The disordered 1D spin chain where spins lie in planes parallel to the plane Λ_0 .*

It is obvious that derivatives of Hamiltonian (15) by angles θ and ϑ are identically equal to zero. Now by equating the expression (16) to zero and solving it, we will get two possible solutions for a stationary point:

$$\begin{aligned}\alpha_{i+1} &= \alpha_i - \arcsin \left[\frac{J_{i-1,i}}{J_{i,i+1}} \sin(\alpha_{i-1} - \alpha_i) \right], \\ \alpha_{i+1} &= \alpha_i + \pi + \arcsin \left[\frac{J_{i-1,i}}{J_{i,i+1}} \sin(\alpha_{i-1} - \alpha_i) \right].\end{aligned}\tag{17}$$

The condition on existence of these solutions in the region of real numbers is equivalent to the following inequality:

$$-1 \leq \frac{J_{i-1,i} \sin(\alpha_{i-1} - \alpha_i)}{J_{i,i+1}} \leq 1, \quad \text{or} \quad |J_{i,i+1}| \geq |J_{i-1,i} \sin(\alpha_{i-1} - \alpha_i)|.\tag{18}$$

Using two equations from (18) and substituting i instead of $i-1$ we can find the value of $J_{i-1,i} \sin(\alpha_{i-1} - \alpha_i)$, and for both solutions result will be same:

$$J_{i-1,i} \sin(\alpha_{i-1} - \alpha_i) = J_{i-1,i} \frac{J_{i-2,i-1} \sin(\alpha_{i-2} - \alpha_{i-1})}{J_{i-1,i}} = J_{i-2,i-1} \sin(\alpha_{i-2} - \alpha_{i-1}).$$

It is clear that by continuing this process we will get:

$$J_{i-1,i} \sin(\alpha_{i-1} - \alpha_i) = J_{1,2} \sin(\alpha_1 - \alpha_2).\tag{19}$$

Using (19) we can transform condition (18) to

$$|J_{i,i+1}| \geq |J_{1,2} \sin(\alpha_1 - \alpha_2)|.\tag{20}$$

Let us note that the angles, α_1, α_2 and also the coupling constant, $J_{1,2}$ in condition (19) as an initial conditions of problem are specified. Finally we can write the condition of the local

minimum energy in the arbitrary i -th node:

$$\frac{\partial^2 H}{\partial \alpha_i^2} = P(\theta, \vartheta) [J_{i-1,i} \cos(\alpha_{i-1} - \alpha_i) - J_{i,i+1} \cos(\alpha_i - \alpha_{i+1})] > 0.$$

IV. THE STATISTICAL ENSEMBLE OF 1D DISORDERED SPIN-CHAINS

As it is easy to verify solutions of equations (5) satisfying the inequalities (8) can be of two types:

a. If $J_{i-1,i} \mathbf{s}_{i-1} \cdot \mathbf{s}_i \leq 0$ and $|J_{i,i+1}| > |J_{i-1,i}|$, then there is only one solution, which we denote by; \mathbf{s}_{i+1}^+ (*queen*), and respectively,

b. If $J_{i-1,i} \mathbf{s}_{i-1} \cdot \mathbf{s}_i > 0$ and $|J_{i,i+1}| \geq |J_{0,1}| \cdot |\mathbf{s}_0 \times \mathbf{s}_1|$, then \mathbf{s}_{i+1}^+ is the solution, in addition there is another solution; \mathbf{s}_{i+1}^- (*drone*) under the condition that, $|J_{i,i+1}| < |J_{i-1,i}|$.

Recall, that the solutions which are denoted with signs "+" and "-" are characterized as follows, if the previous solution is the *queen* "+", then it is possible to find up two different solutions \mathbf{s}_{i+1}^+ and \mathbf{s}_{i+1}^- , while after the *drone* "-" the solution only one \mathbf{s}_{i+1}^+ . Taking into account this we can construct solutions graphically in the form of separate *Fibonacci subtrees* (\widehat{FsT}_i) (see Fig. 2).

The mathematical expectation of the branching depending on the height of \widehat{FsT}_i can be calculated by the following formula:

$$M(n) = M(n-1) \lfloor (2\xi_n) \rfloor = \lfloor 2^{n\eta(n)} \rfloor, \quad \eta(n) = 1 + n^{-1} \sum_{k=1}^n \log_2(\xi_k) > 0, \quad (21)$$

where $M(n-1)$ the number of the branching at the height $(n-1)$, while ξ_k denotes a random coefficient which belongs to the interval $[1/2, 1]$. Note, that for simplification of the formula (21) designating the subtree's number i is omitted. Since, an each \widehat{FsT}_i consists of the set of nodes and the set of edges (the set of constants $\{J\} = [J_{1,2}, J_{2,3}, \dots, J_{n-1,n}]$ therefore it can be represented as a graph $G_i(n) \cong \{g_j(n), j \in M\}$, where $g_j(n)$ denotes a random string by length n which is characterized by Kolmogorov's complexity^{23,24}.

Note that each Fibonacci subtree (graph) depending on its height n can be represented itself as a random process. For their comparing we can formulate the following criterion:

Definition. Two graphs with the same height; $G_1(n)$ and $G_2(n)$ are equivalent with a given accuracy $O(\epsilon)$, where $\epsilon \ll 1$, if the following conditions take place:

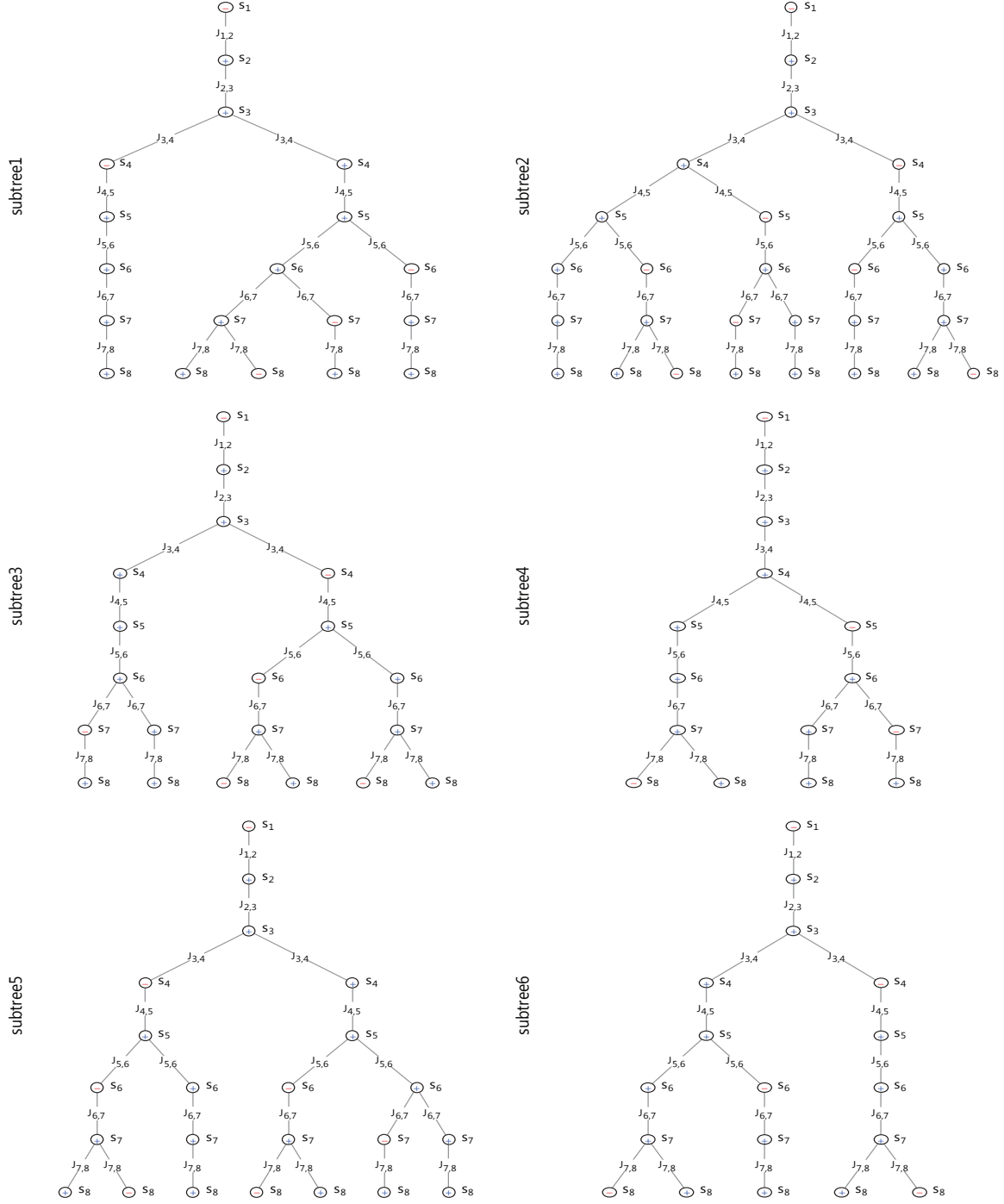


FIG. 2. The six different Fibonacci subtrees (graphs) with the height 8. All these graphs are growing from the same initial data (root) in result of the six independent numerical experiments. Note, that the same symbols s_i and $J_{i,j}$ on different graphs can have completely different values.

1) The difference of Shannon's entropy of the two Fibonacci subtrees (graphs) satisfies:

$$|S^1(n) - S^2(n)| \leq \epsilon, \quad S^{1(2)}(n) = - \sum_{i=1}^n M_i^{1(2)} \ln M_i^{1(2)}, \quad (22)$$

where $S^1(n)$ and $S^2(n)$ denote the Shannon's entropies of graphs $G_1(n)$ and $G_2(n)$, in addition M_i^1 and M_i^2 are the branching numbers of corresponding graphs on the i -th height,

2) the difference of average polarizations of two graphs in per one spin satisfies:

$$\left\| \frac{1}{n} \sum_{i=1}^n (\mathbf{s}_i^{(1)} - \mathbf{s}_i^{(2)}) \right\| \leq \epsilon, \quad (23)$$

where $\mathbf{s}_i^{(1,2)} = \sum_{G_{1,2}(i)} \mathbf{s}_i$ denotes the total value of spins on the corresponding graph at the i -th height,

3) the difference of the average energies of two graphs in per one spin satisfies:

$$\frac{1}{n} \sum_{i=1}^n \left| \frac{1}{m_1} \sum_{j=1}^{m_1} J_{i,i+1;(j)}^{(1)} \mathbf{s}_{i;(j)} \mathbf{s}_{i+1;(j)} - \frac{1}{m_2} \sum_{j=1}^{m_2} J_{i,i+1;(j)}^{(2)} \mathbf{s}_{i;(j)} \mathbf{s}_{i+1;(j)} \right| \leq \epsilon, \quad (24)$$

where $m_1 = M_n^1$ and $m_2 = M_n^2$.

In the case when at least one condition from (22)-(24) is violated, we will consider that $G_1(n)$ and $G_2(n)$ are inequivalent or independent.

Thus, for calculations of different physical parameters of the statistical ensemble, it is necessary to take into account the contribution of all independent graphs (set of graphs) $\{G(n)\}_N = [G_1(n), \dots, G_i(n), \dots]$, where $i = \overline{1, N}$ and N the number of graphs.

As mentioned above, the system of equations (5) which satisfies conditions (8)-(9) in each node can have up to two solutions. The latter means that the number of solutions on the step n due to branching will be of order $M(n) \propto 2^n$ and correspondingly, the calculation problem of the statistics even of one graph algorithmically is a NP hard problem, since at increasing of spins number the number of solutions grows exponential.

Evaluation of the computational complexity of the statistics for a single graph gives:

$$K_t(n) \propto M(n) K_s(n), \quad (25)$$

where $K_s(n)$ denotes the Kolmogorov complexity of the string $g_j(n)$, while $K_t(n)$ denote the complexity of the graph $G_i(n) \subset \{G(n)\}_N$. The computational complexity of the ensemble, which is represented as the set $\{G(n)\}_N$, obviously will be order; $K_{ens} \propto NM(n) K_s(n)$.

The mathematical expectation of random variable f characterizing the ensemble $\{G(n)\}_N$ can be calculated by the formula:

$$E[f] = \bar{f} = \frac{\sum_{i=1}^N w_i \bar{f}_i}{\sum_{i=1}^N w_i}, \quad w_i = N_i / \bar{N}, \quad (26)$$

where N_i and \bar{N} denote the number of strings of the graph $G_i(n)$ and the total number of strings in the ensemble respectively, in addition $\bar{f}_i = \sum_{G_i(n)} f$ denotes the expectation of a random variable f on the $G_i(n)$, which is calculated similarly to formula (26).

From the point of view of statistics, it is important to investigate the ensemble in the state of the statistical equilibrium. This as a rule is realized at $N \gg 1$ and when the average value of random variable f almost surely converges to the expected value²⁵:

$$\Pr\left(\lim_{N \rightarrow \infty} \bar{f}_N = \bar{f}\right) = 1,$$

where f_1, f_2, \dots are infinite sequence of Lebesgue integrable random variables with the expected values $E[f_1] = E[f_2] = \dots = \bar{f}$.

Lemma. *If statistical weights of all independent graphs $G_i(n) \subset \{G(n)\}_N$ are approximately the same it can be shown that the statistical weights of all strings $g_j(n) \subset \{G(n)\}_N$ are equal exactly. In this case we can use the law of large numbers and simplify the expression (26) writing it as:*

$$E[f] = \bar{f} = \frac{1}{N} \sum_{j=1}^N \tilde{f}_j + O(N^{-1/3}), \quad (27)$$

where $\tilde{f}_j = \sum_{g_j} f$ denotes the expectation of the random variable f on a randomly selected string $g_j(n) \subset G_i(n)$.

Note that the asymptotic convergence to the limit value in the expression (27) occurs with accuracy $\propto N^{-1/3}$ due to the fact that the spins are three-dimensional.

Thus, the computation of statistical parameters of the disordered spin system by the formula (26) is algorithmically equivalent to solving of NP hard problem (the left scheme in Fig. 3). In the case when the ensemble is in the state of statistical equilibrium then the numerical simulation can be realized by the formula (27) and respectively by the algorithm P (the right scheme in Fig. 3) having the polynomial complexity.

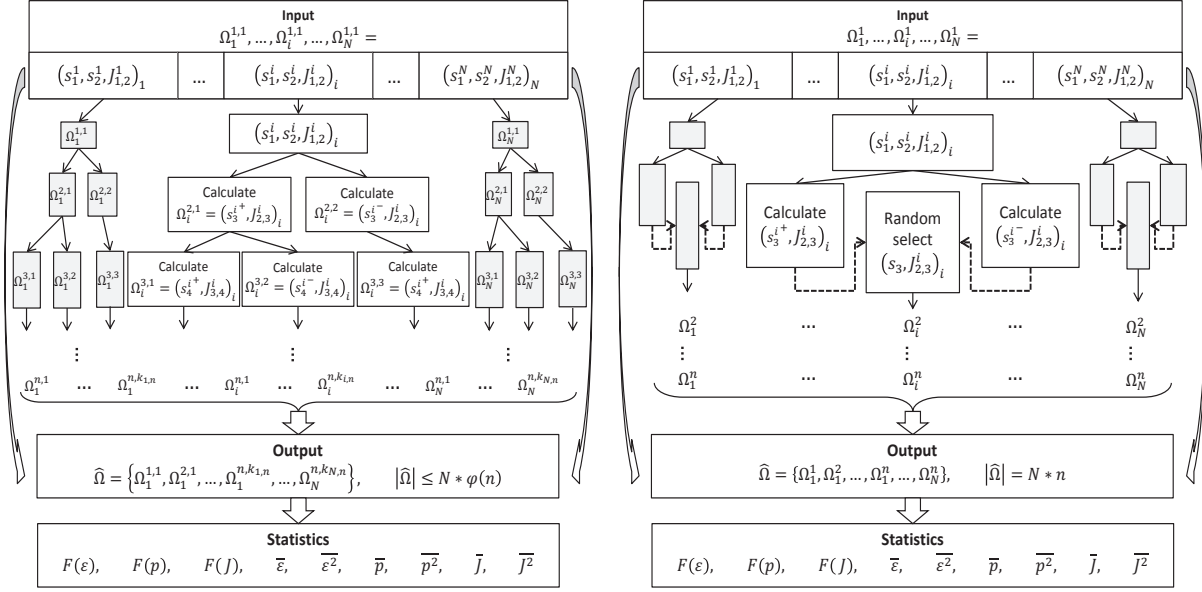


FIG. 3. The left scheme describes algorithm, which allows to sort out all graphs of the ensemble and, correspondingly, this algorithm in the future will be called \mathbb{NP} algorithm, while the right one describes \mathbb{P} algorithm which allows implementing calculations of the problem in a polynomial time.

V. THE NUMERICAL EXPERIMENTS

As it has been said, usually the problems of spin glasses are studied in the framework of the partition function representation by using Monte Carlo simulation methods, which however does not allow to answer on many important questions of the statistical ensemble. In particular, is an important problem is that the spin glass in the state of a statistical equilibrium generally speaking is in a metastable state and has some distribution near the *ground state*, while Monte Carlo simulation methods are adapted for calculations only the *ground state*. It is clear, that the influence and contribution of this distribution on different properties and values of parameters of a spin glass may be accounted, if the numerical simulation of the spin system to spend from first principles of classical mechanics.

Hypothesis. *If the Heisenberg 1D spin glass is in the state of the statistical equilibrium, then the computational \mathbb{NP} hard problem with the prescribed accuracy ϵ can be reduced to the \mathbb{P} problem.*

It should be noted that at performing of numerical simulations with the same initial data, everytime "t" we find a new set of graphs $\{G(n)\}_N^t$ (see Fig. 2), nevertheless we expect that

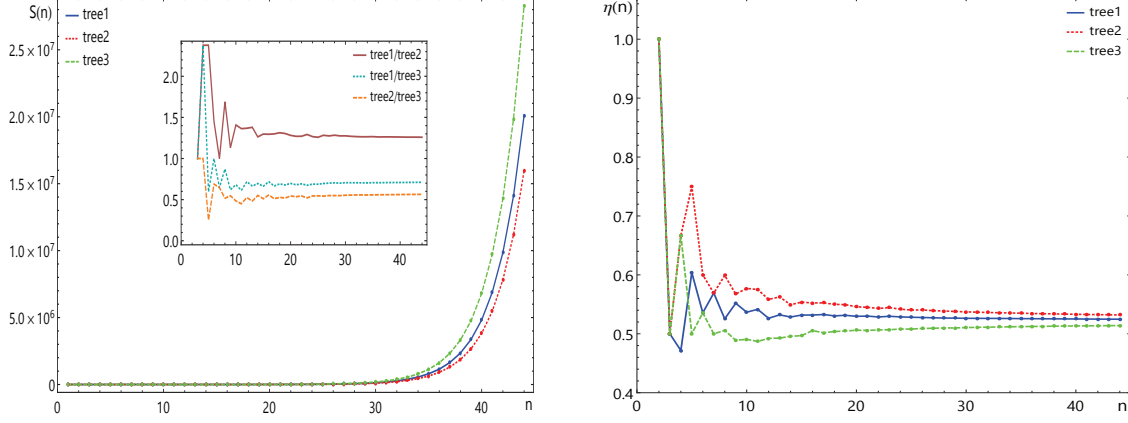


FIG. 4. In the left figure are shown the entropies of graphs (subtrees) depending on their height (the red, blue, and green lines), while in the small frame are shown curves of relations of corresponding entropies. In the right figure are shown curves of the branching factor $\eta(n)$ of different graphs depending on their height.

in the limit of statistical equilibrium all these sets must be identical in terms of statistical properties $\{G(n)\}_N^{t_0} \propto \{G(n)\}_N^{t_1} \dots \propto \{G(n)\}_N^{t_n}$ and this is the assumption of the hypothesis. It is obvious, if we prove that all strings in the statistical ensemble $\{G(n)\}_N$, have the equal weight then this allows to use the law of big numbers and to reduce NP hard problem to P problem with the prescribed accuracy.

For a detailed study of the properties of graphs and their contributions to the statistics of the ensemble, we will consider two possible cases; when graphs are growing from one single *root* and, respectively, when they grow from different *roots*.

At first let us consider one set of initial data Ω_i^1 (root) which includes orientations of the first two spins of the chain and the coupling constant between them which are generated randomly from the corresponding homogeneous distributions. Using the system of recurrence equations (5), with consideration of inequality conditions (8), we perform successive calculations of spin-chain. Recall that this system of equations connects three consecutive spins, so that knowing the configuration of two previous spins, we can generate from log-normal distribution²⁶ a random constant $J_{i,i+1}$ and exactly to calculate the orientation of the spin in the subsequent node. Conducting the consecutive node-by-node calculations on the n -th step, we generate a random graph $G_i(n) \subset \{G(n)\}_N$ at internal nodes of which spins are in local minima of energies. With regard to the spins in the external nodes, it is

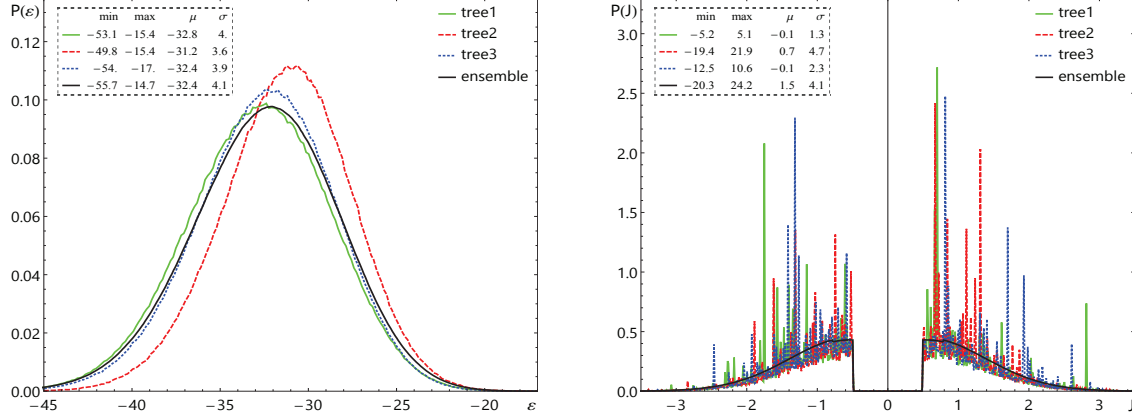


FIG. 5. On the left picture are shown the distributions of strings' energies of the length 45 in the three different graphs (red, green and blue lines) which grow from the same root and correspondingly the black curve, which shows the energy distribution in statistically equilibrium ensemble $\{G(n)\}_N$, where all graphs from one root are growing. In addition, in tables adduced the important parameters that characterize the corresponding distributions; the maximal and minimal values, the average value of parameter $\mu = \int xP(x)dx$ and the dispersion σ . Note that the simulation has been conducted by NP algorithm (see the left scheme on Fig. 3).

assumed that they satisfy the conditions of local minima of energy, on the basis of other considerations.

The simulation using the NP algorithm shows, that all three graphs which *grow* from one *root* are independent, by the criteria (22)-(24). In particular the numerical simulations show that depending on height of the graph, the Shannon's entropy *grows* an exponential, in all cases starting with $n \simeq 15$ (see the left picture on Fig. 4). The ratios of entropies, as shown in Fig. 4, for the $n > 15$ take values $\propto O(1)$ that means in the ensemble $\{G(n)\}_N$ the weights of separate graphs are approximately equal. The weight of individual branches in the statistical ensemble obviously will be the inverse of weights of graphs to which they belong. In other words all branches in the ensemble have the same weight. Note that the same picture is observed when graphs are *growing* from different *roots*. In this case all graphs are also independent and the parameter of branching, at increasing of string length as in the previous case converges to the value $\eta(n) = 0.55$ (see the right picture on Fig. 4). When the length of string $n < 15$ then in the behaviour of entropy an oscillating character is observed (see Fig. 4), that is characteristic of the discrete systems and manifests itself as a

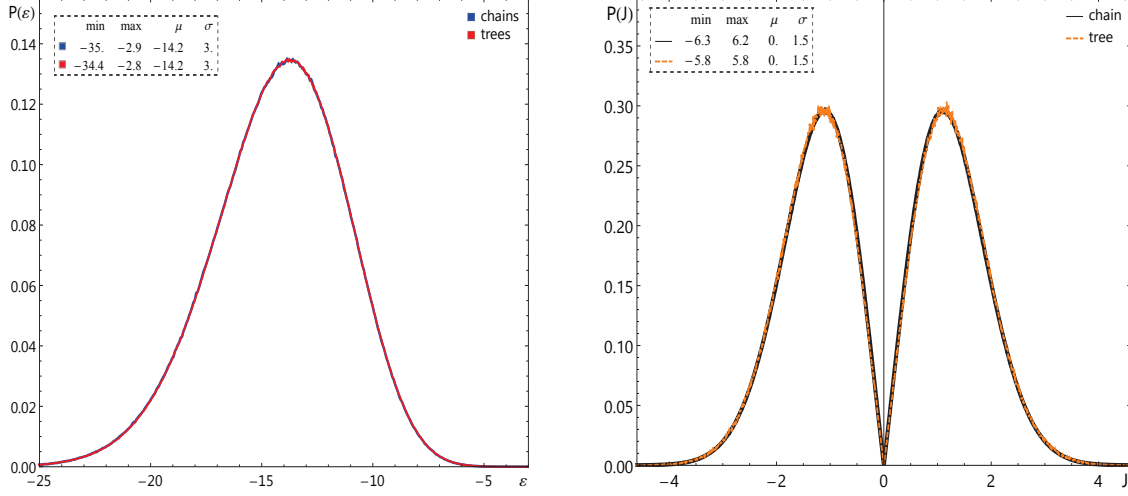


FIG. 6. The distributions of energies and spin-spin coupling constant. The black curves denote the results of calculations using \mathbb{P} algorithm, while beige curves are constructed in result of calculations by \mathbb{NP} algorithm.

size effects. We carried calculations of distributions of different parameters on the example of three graphs and also of the ensemble of graphs which *grow* from the same *root*. As the calculations show, the energies distributions for three graphs and the ensemble, $\{G(n)\}_N$ by criterion of Kullback-Leibler distance are close enough²⁷, while distributions of the spin-spin coupling are sufficiently far, by the same criterion (see Fig. 5).

So, we have shown that there are necessary and sufficient conditions for performing of the **lemma**.

Now we will prove the **hypothesis** on the example of numerical experiments. The characteristic distributions and parameters of the 1D spin glass, which is in the state of the statistical equilibrium will be calculated using two \mathbb{NP} and \mathbb{P} algorithms. It is obvious that the comparison of the simulation results of the relevant distributions will allow us to prove or disprove the **hypothesis**.

For simulation of the problem, first of all we have to set the initial conditions in the form of a large number of independent configurations (roots); $\{\Omega_1^1 = (\mathbf{s}_1^1, \mathbf{s}_1^1; J_{1,2}^1), \dots, \Omega_N^1 = (\mathbf{s}_1^1, \mathbf{s}_2^1; J_{1,2}^1)_N\} = \hat{\Omega}$ (see the two scheme on Fig. 3).

Stages of simulation using of the algorithm \mathbb{NP} are as follows (the left scheme on Fig. 3). Using the initial data, $\hat{\Omega}$ we perform parallel calculations of all graphs $G_i(n)$ of the ensemble $G_i(n) \subset \{G(n)\}_N$. Note that each of these graphs in terms of classical mechanics,

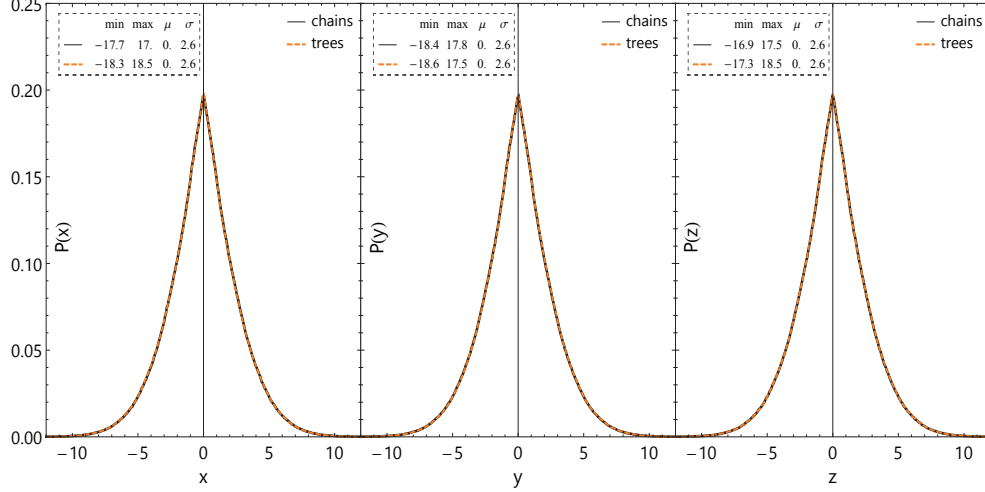


FIG. 7. The distributions of polarizations in the ensemble of spin-chains by axes, which are calculated using \mathbb{NP} (beige curves) and \mathbb{P} (black curves) algorithms.

represents itself the set of classical trajectories that go out from one initial value (*root*). The database, which is obtained in result of simulation using \mathbb{NP} algorithm allows to construct the distributions of the basic parameters of the statistically equilibrium ensemble.

The simulation using \mathbb{P} algorithm (the right scheme on Fig. 3), is performed in a similar way, but with the difference that in this case instead of the set of graphs $\{G(n)\}_N$ we *grow* the set of strings $\{g(n)\}_N$. In this case in the each graph we choose only one string as the *representative*. Note, that the string (branch) $g_j(n) \subset \{G(n)\}_N$ we grow by way of randomly selecting only one solution in each node. As a result of parallel simulation of the set of strings, we get the database which allows to construct all distributions of the statistically equilibrium ensemble, $\{G(n)\}_N$ with the asymptotic accuracy $O(N^{-1/3})$.

We compared results of numerical simulations on the example of the statistical ensemble, $\{G(20)\}_{5 \cdot 10^4}$ consisting of $5 \cdot 10^4$ graphs by heights 20 with the ensemble $\{g(20)\}_{5 \cdot 10^4}$, which consists from the $5 \cdot 10^4$ strings of lengths 20. As can be seen from Fig. 6 and Fig. 7, in the limit of statistical equilibrium, the distributions of various parameters of the statistical ensemble that have calculated using of two \mathbb{NP} and \mathbb{P} algorithms coincide ideal.

Thus we have shown on the example of 1D Heisenberg spin glass, that the \mathbb{NP} hard problem with given accuracy may be reduced to the \mathbb{P} problem and respectively the **hypothesis** is proved.

VI. PARTITION FUNCTION

Now it is important return to the definition of the basic object of statistical physics, i.e., to the partition function.

As well known, the multiparticle classical system in the state of statistical equilibrium in the configuration space is described by the partition function of type:

$$Z(\beta) = \int \dots \int \exp\{-\beta \mathcal{H}(\{\mathbf{r}\})\} d\mathbf{r}_1 \dots d\mathbf{r}_N, \quad \beta = 1/k_B T, \quad \{\mathbf{r}\} = (\mathbf{r}_1, \dots, \mathbf{r}_N), \quad (28)$$

where $\mathcal{H}(\{\mathbf{r}\})$ is the Hamiltonian of the system in the configuration space, k_B and T are the Boltzmann constant and temperature of the system respectively.

For the considered model the partition function is calculated exactly²¹:

$$Z(\beta, \{J\}) = \prod_{i=1}^n \frac{\sinh(a_i)}{a_i}, \quad a_i = \beta J_{i,i+1}, \quad (29)$$

where the coupling constants; $J_{i,i+1} \in \{J\} = (J_{1,2}, J_{2,3}, \dots, J_{n-1,n})$ are a random variables.

The average value of the partition function for the ensemble may be found by averaging over the distribution of the coupling constant. Note that often assumed that this distribution is Gaussian:

$$W(J) = \frac{1}{\sigma_J \sqrt{2\pi}} \exp\left\{-\frac{(J - J_0)^2}{2\sigma_J^2}\right\}, \quad (30)$$

where σ_J is the variance and J_0 is the average value of coupling constant.

After averaging of the expression (29) by the distribution (30) it is easy to find:

$$\bar{Z}(\beta) = \int_{-\infty}^{+\infty} Z(\beta, \{J\}) W(J) dJ = \frac{K(\beta)}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{\sinh(\sigma_J \beta x)}{\sigma_J \beta x}\right)^n \exp\left\{-\frac{1}{2}(x - x_0)^2\right\} dx, \quad (31)$$

where $x = J/\sigma_J$ and $x_0 = J_0/\sigma_J$, in addition $K(\beta)$ denotes the normalization factor of the partition function:

$$K^{-1}(\beta) = \frac{1}{2\bar{J}} \int_{-\bar{J}}^{+\bar{J}} \left(\frac{\sinh(J\beta)}{J\beta}\right)^n dJ = \frac{1}{\bar{y}} \int_0^{\bar{y}} \left(\frac{\sinh(y)}{y}\right)^n dy, \quad \bar{y} = \bar{J}\beta, \quad J \in [\bar{J}, -\bar{J}],$$

Recall that the coefficient $K(\beta)$ is constructed in such way that the Helmholtz free energy in the limit $\beta \rightarrow \infty$ converges to zero.

The Helmholtz free energy per one spin in chain is calculated as follow:

$$F(\beta) = -\frac{1}{n\beta} \ln \bar{Z}(\beta). \quad (32)$$

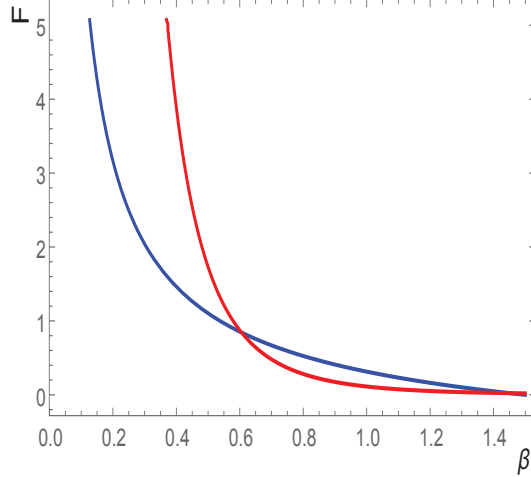


FIG. 8. The free energy of the ensemble which is calculated by two methods. The red curve is obtained at using of the expression (33), while the blue curve is obtained in the result of calculation by the expression (32). Note that parameters of ε_0 and σ_ε are found by the way of simulation of problem from first principles, whereas parameters J_0 and σ_J chosen on the basis of the best approximation to the red curve.

Since the integration in the representation (28) is carried out by the full configuration space, then obviously in such way taken into account also contributions of spin configurations, which physically are unrealizable. Let us note that usually, the measure of set of such spin configurations is assumed to be equal to zero without any serious proof, that not only groundlessly but in a number of cases may be incorrect. Taking into account the fact that the set of strings describing the statistical ensemble in configuration space formally can be represented as a trajectory of dynamical system, in the limit of ergodicity of system (see [27, 28]), for the partition function the following representation may be written:

$$Z_*(\beta) = \int_{-\infty}^{-n/\beta} \bar{P}(\varepsilon) d\varepsilon, \quad \bar{P}(\varepsilon) = c^{-1} P(\varepsilon), \quad c = \int_{-\infty}^0 P(\varepsilon) d\varepsilon, \quad (33)$$

where $\varepsilon < 0$ denotes the energy of 1D spin-chain, while $\bar{P}(\varepsilon)$ is the normalized distribution of energy of the ensemble. Recall that $-n/\beta$ denotes the limit of energy, above which there can be no stable spin-chain. As for the lower limit then it should be $-\infty$, since on idea for all negative values of energies exist a stable spin-chain configurations, nevertheless as seen from Fig. 6, starting from the value $\varepsilon_0 = \mu$ (the average value of the spin-chain energy) with decreasing of the energy the probability of formation of spin-chains decreases.

If the energy distribution (see Fig. 6) to approximate by the Gaussian function (see (30)) then using the representation (33), for the free energy attributable to a single spin can be found the following expression:

$$F_{\star}(\beta) = -\frac{1}{n\beta} \ln \left\{ \frac{1}{2} \left[1 - \operatorname{erf} \left(\frac{\varepsilon_0 + n/\beta}{\sqrt{2}\sigma_{\varepsilon}} \right) \right] \right\}, \quad (34)$$

where $\varepsilon_0 = \mu < 0$ (see Fig. 6) denotes the average energy of spin-chain in the ensemble and σ_{ε} , respectively, denotes the variance of spin-chains' energy distribution. Comparing Helmholtz's free energies, $F(\beta)$ and $F_{\star}(\beta)$ for the ensemble $\{g(20)\}_{5 \cdot 10^5}$ shows, that already at finite temperatures these curves diverge significantly (see Fig. 8). Furthermore, near the temperature $\beta \simeq 0.3$, the ensemble of spin-chains exhibits a critical behavior, since the free energy tends to infinity that is characteristic at phase transitions of first order. The latter obviously connected with taking into account of contribution non-physical configurations in the representation (28), and in formulas (29) and (30) respectively.

VII. CONCLUSION

We have studied 1D spin glass in the framework of Heisenberg's nearest-neighboring Hamiltonian (1). Using (1) we obtained the system of recurrent algebraic equations (4), which together with conditions of energy minimum in nodes (6) allow to implement node-by-node calculations and to construct stable spin-chains. It is proved, that in the considered model, the system of spins form only such spin-chains where all spins lie in one plane, while these planes relative to each other may have any angle. Another important feature of the system of equations (4) consists in that there are probability of branching of solution in each node of 1D lattice. This leads to the fact that in result of consecutive calculations, from the one initial condition (*root*) on the n -th step, we get a set of solutions (stable spin-chains or Kolmogorov's strings $g_i(n)$) that form the *Fibonacci subtree* (random graphs $G_j(n) \supseteq g_i(n)$). In other words, when we say on the statistical ensemble we mean the set of random graphs $\{G(n)\}_N$, where N denotes number of graphs in the ensemble and correspondingly the problem consists in that to calculate all parameters and corresponding distributions characterizing the ensemble.

It is shown that the computational complexity of arbitrary graph $G_j(n)$ is the \mathbb{NP} hard problem of the order $2^n K_s(n)$, while complexity of the ensemble, with increasing number of

elements is increases linearly, $\{G(n)\}_N$ is the $\sim 2^n N K_s(n)$. The properties of random graphs depending on their height are studied in detail (see Figs 4-5) by using \mathbb{NP} algorithm (see the left scheme on Fig. 3) and conditions at which the ensemble $\{G(n)\}_N$ is in the state of the statistical equilibrium are formulated. We analyzed and proposed the hypothesis that the $1D$ spin glass in the limit of statistical equilibrium may be simulated by using \mathbb{P} algorithm (see the right scheme on Fig. 3). Let us note, that all theoretical results and predictions have been confirmed with high accuracy in numerical experiments that have been performed using \mathbb{NP} and \mathbb{P} algorithms (see Figs 5-7). It is noteworthy that the simulation by the algorithm \mathbb{P} not only ensures high precision but also allows to find distributions of all parameters of the ensemble, including the distribution of a constant spin-spin coupling (see Fig. 5).

In the work has been suggested a new representation for the partition function in the form of one dimensional integral from the spin-chain's energy distribution (see the expression (33)). We compared the Helmholtz free energies, which was calculated by using the usual (32) and new (34) representations. As it is shown (see Fig. 8), already at finite temperatures the corresponding curves significantly different, moreover near $\beta \sim 0.3$ the ensemble of spin-chains demonstrates critical property, that usually occurs at first order phase transitions. This is obviously due the fact that in the formula (31), only such spin configurations are counted which satisfy to the basic principles of classical mechanics (see expressions (4) and (6)).

Thus, the main advantages of developed approach are that we have received clear answers, to all raised questions on the example of study $1D$ spin glass from first principles of the classical mechanics without using any additional assumptions. We showed that in the limit of statistical equilibrium (at ergodicity of the statistical system), the initial \mathbb{NP} hard problem is reduced to the \mathbb{P} problem, that allows radically simplify the simulation of spin glasses.

The ideas lying in the base of developed approach enough are universal and allow the generalization of model for a multidimensional case and at presence of external fields³⁰.

Finally, a new formulation of the problem of spin glasses and disordered systems in general can be very useful for study of a global problem, i.e the problem of reduction \mathbb{NP} to the \mathbb{P} .

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